LESLIE A. KUHN

Curriculum Vitae

Education

University of California, Los Angeles, CA, major in Biochemistry, 1977–1980
University of Pennsylvania, Philadelphia, PA, B.A. in Computer Mathematics, 1984
University of Pennsylvania, Philadelphia, PA, Ph.D. in Biophysics, 1989

Professional Experience

Postdoctoral Research Fellow, The Scripps Research Institute, La Jolla, CA, June 1989–August 1992
Research Associate, The Scripps Research Institute, La Jolla, CA, September 1992–April 1994
Assistant Professor, Department of Biochemistry, Michigan State University, East Lansing, MI, May 1994–April 2000
Adjunct Assistant Professor, Department of Physics and Astronomy, Michigan State University, East Lansing, MI, April 1999–April 2000
Co-Founder and Research Scientist for MolFlex, a biotechnology software company, 1997–1999
Research Consultant, AstraZeneca Research & Development, Charnwood, UK, 1999–2000
Senior Scientist, Computational Chemistry, Pfizer Global Research and Development, La Jolla, CA, 2002 (during leave of absence from MSU)
Associate Professor, Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI, May 2000–May 2004
Adjunct Associate Professor, Department of Physics and Astronomy, Michigan State University, East Lansing, MI, May 2000–May 2004
Founding Director, Research Excellence Fund Center for Biological Modeling, MSU, 2000–2001 and 2003–2004
Co-Director, Quantitative Biology and Modeling Initiative, Michigan State University East Lansing, July 2004–November 2007
Adjunct Professor, Department of Physics and Astronomy, Michigan State University, East Lansing, MI, June 2004–June 2013
Consultant, Dart NeuroSciences, 2012
Adjunct Professor, Department of Fisheries and Wildlife, Michigan State University, East Lansing, MI, June 2013–June 2016
Professor, Computer Science and Engineering, MSU, July 2005–August 2019
Professor, Department of Biochemistry and Molecular Biology, MSU, June 2004–August 2019

Inventions, Database Submissions, and Software

"Glycosaminoglycan-Targeted Fusion Proteins, Their Design, Construction and Compositions", John A. Tainer, Leslie A. Kuhn, Maurice Boissinot, Cindy L. Fisher, Hans E. Parge, John H. Griffin, Guy T. Mullenbach, and Robert A. Hallewell. United States patent application 07/608,569 (11/90); EPC (Europe), Australia, Canada, Japan, and Korea (11/91).
"Receptor Internalization Signals", Ian S. Trowbridge, James F. Collawn, John A. Tainer, and Leslie A. Kuhn. United States patent application 07/844,852 (3/92).

Coordinate sets deposited in the Protein Data Bank: 4SOD: Heparin-Binding Superoxide Dismutase; 1PAI and 2PAI: Protein C Inhibitor Homology Models

Surfractal, *MaxAccess*, and *SrftoBiosym* protein surface analysis software distributed via the NSF Computational Center for Macromolecular Structure, San Diego Supercomputer Center (1993) Leslie Kuhn, Michael E. Pique, Craig A. Swanson, John A. Tainer, and Elizabeth D. Getzoff

Consolv water-mediated ligand binding prediction software, database, documentation, and test cases distributed via Software category at http://www.kuhnlab.bmb.msu.edu (1998) Michael L. Raymer, Paul C. Sanschagrin, Vishal Thakkar, and Leslie Kuhn

Sequery and SSA software for predicting peptide conformation, distributed via Software category at http://www.bch.msu.edu/labs/kuhn (1999) Paul C. Sanschagrin, Michael E. Pique, Michael A. Siani, John A. Tainer, Elizabeth D. Getzoff, Tharuna Niranjan, and Leslie Kuhn

WatCH software for identifying conserved water sites in series of molecular structures, distributed via the Software category at http://www.bch.msu.edu/labs/kuhn (2001) Paul C. Sanschagrin and Leslie A. Kuhn

SLIDE software for screening and docking flexible ligands from molecular databases to flexible, solvated proteins; distributed by licensing from Michigan State University (2000-Present) Volker Schnecke, Paul C. Sanschagrin, and Leslie A. Kuhn

MSU ProFlex and ROCK software for predicting flexible regions in proteins, made available as source code by licensing from Michigan State University (2002-Present) Donald J. Jacobs, Andrew J. Rader, Brandon M. Hespenheide, Leslie A. Kuhn, and Michael F. Thorpe

International and U.S. Patent Applications with Agouron Pharmaceuticals, Pfizer Global Research and Development, La Jolla, CA (U.S. Patent Office 60/361,645, March 4, 2002 and 60/432,275, December 9, 2002; European Patent Office 03702902.2-2107-IB0300615, February 17, 2003) on "Combination Therapies for Treating Methylthioadenosine Phosphorylase Deficient Cells"

U.S. Patent Application with Michigan State University co-authors David Wenkert, Erica Scheller, Michael Kron, and Yuehai Shen, February 2006, on "Parasitic Heat Shock Protein Inhibition by Ansamycin and Radicicol Derivatives"

SimSite3D software for identifying non-homologous sites that bind similar small molecules; developed by Jeffrey Van Voorst and Leslie Kuhn, installed globally at Pfizer Research & Development and distributed by GitHub (2010-Present)

StoneHinge software for identifying protein domains and hinges, made available by web server and downloading from stonehinge.bmb.msu.edu (2009-2015); developed by Kevin Keating, Samuel Flores, Mark Gerstein and Leslie Kuhn

CholMine software at cholmine.bmb.msu.edu for predicting cholesterol and cholate binding sites on proteins; developed by Nan Liu, John Johnston, and Leslie Kuhn (2014-Present)

SiteInterlock software for predicting protein-small molecule interactions based on interfacial rigidification, developed by Sebastian Raschka and Leslie Kuhn; https:/psa-lab.github.io/siteinterlock/index.html (2016–Present)

Screenlamp software developed by Sebastian Raschka and Leslie Kuhn; https://github.com/psa-lab (2018–Present)

Protein Recognition Index, Hbind, and HbindViz software developed by Sebastian Raschka and Leslie Kuhn; https://github.com/psa-lab (2018–Present)

SpeciFlex software by Matthew Tonero and Leslie Kuhn; defines volumes sampled by atoms in MD trajectories or across multiple crystal or NMR structures; also computes difference volumes from two trajectories or conformational ensembles; https://github.-

com/psa-lab (2018–Present).

Protein Alignment Tool software by Joseph Bemister-Buffington and Leslie Kuhn; takes Dali residue correspondences from 3D structural alignment of proteins, producing a formatted alignment of binding site residues or numeric properties from PDB B-value columns; https://github.com/psa-lab (2019–Present).

Grants and Awards

Regents Scholarship, University of California, Los Angeles

Alumni Scholarship, University of California, Los Angeles

N.I.H. Postdoctoral Training Grant, June 1989–May 1990

National Cancer Institute N.R.S.A. Individual Postdoctoral Fellowship, September 1990–September 1992

American Cancer Society, California Division Senior Postdoctoral Fellowship, September 1992–April 1994

M.S.U. Cancer Center Grant, "Nuclear Targeting in Colon Cancer", Co-Investigator (John Wang and William Smith, PI's), January 1995–December 1996

M.S.U. AURIG Grant, "Water in Molecular Recognition and Protein Inhibitor Design", Principal Investigator, May 1995–August 1996

Research Excellence Fund Center for Protein Structure, Function, and Design Grant, "Evaluating the Favorability of Drug Candidates for Protein Inhibition", Principal Investigator, July 1995–June 1997

American Heart Association Grant-in-Aid, "Decoding Functionally Required Residues in Prostaglandin Synthase", Principal Investigator, July 1996 – June 1997

National Institutes of Health Program Project Grant, "Oxygen Utilizing Membrane Heme Proteins: Substrate Docking in Cytochrome c Oxidase", Co-Principal Investigator (Shelagh Ferguson-Miller, project PI; William Smith, program PI), June 1998–May 2003

National Institutes of Health Grant, "Mosquito Oocytes–Mechanism of Protein Accumulation", Co-Principal Investigator (Alexander Raikhel, PI), June 1997–May 2002

American Heart Association Grant-in-Aid, "Defining the Role of Bound Water in Thrombin Specificity", Principal Investigator, July 1997–June 1998

Research Excellence Fund Center for Protein Structure, Function, and Design Grant, "The Rigid Regions in Macromolecules", Co-Principal Investigator (Michael F. Thorpe, Co-PI), July 1997–June 1998

National Science Foundation Early Career Development Award, "Resolving Protein–Water Recognition", Principal Investigator, August 1996–July 2001

Postdoctoral Sponsor, Deutsche Forschungsgemeinschaft Postdoctoral Fellowship to Volker Schnecke, "Distance Geometry and Genetic Algorithms in Molecular Screening and Docking", June 1997–May 1999

Research Excellence Fund Center for Protein Structure, Function, and Design Grant, "Flexible Regions in Proteins", Co-Principal Investigator (Michael F. Thorpe, Co-PI), July 1998–June 1999

National Institutes of Health Small Business Innovation Research Grant, "Real-Time Protein Domain and Flexibility Identification", Research Scientist (Donald J. Jacobs, PI), 1998–1999

American Heart Association Established Investigator Grant, "Phage-display and Computational Peptide Library Screening for Coagulation Inhibitors", Principal Investigator, January 1999–December 2003

Research Excellence Fund, MSU Center for Biological Modeling grant, Principal Investigator, July 2000–June 2004

National Institutes of Health Mathematics in Biology grant, "New Algorithms for Modeling Flexibility in Proteins", Principal Investigator, Michigan State University subcontract, July 2002–June 2006

National Institutes of Health Partnership for Novel Therapeutic, Diagnostic, and Vector Control Strategies grant, "Macrofilaricidal Aminoacyl-tRNA Synthetase Inhibitors", Co-Principal Investigator (Michael A. Kron, PI), September 2002 – August 2007

Michigan State University Foundation Strategic Partnership Grant, "Quantitative Biology and Modeling Initiative", Leslie Kuhn, Principal Investigator (Shelagh Ferguson-Miller and Robert Cukier, Co-PI's), July 2004–June 2007

Pfizer Strategic Alliance Grant, "ASCbase", Leslie Kuhn, Principal Investigator, December 2005–November 2010

Great Lakes Fishery Commission Grant, "Development of a 3kPZS Antagonist for Sea Lamprey Control", Leslie Kuhn, Principal Investigator (Weiming Li, Co-PI), January 2012–December 2015

Great Lakes Fishery Commission Grant, "Development of Antagonists to Pheromonal Sulfated Steroids for Sea Lamprey Control", Leslie Kuhn, Principal Investigator (Weiming Li, Co-PI), January 2015–December 2017

National Institutes of Health R01 Grant, "Schlafen Mediation of Intestinal Differentiation", Co-Principal Investigator (Marc Basson, PI), September 2014–September 2018

Department of Defense Peer Reviewed Orthopaedic Research Program Grant, "Enhancing Notch Activation for Improved Bone Regeneration", Leslie Kuhn, Co-Principal Investigator (Kurt Hankenson, Principal Investigator), Sept. 30, 2015–Sept. 29, 2018

Professional Service Outside MSU

Program Committee for Genetic Programming 1997 and 1998 Conferences, Stanford University

Advisory Committee for Rigidity Theory and Applications Interdisciplinary Workshop, 1998

N.I.H. Computational Biology Research Resource Site Visitor, July 1999

Organizer (with Michael Thorpe) of Workshop on Protein Folding, Traverse City, Michigan, August 2000

N.I.H. Structural Genomics Study Section, November 2000

General Series Editor, *Biological Modeling*, Elsevier

Chair, Global Working Group on Structure-Based Ligand Docking, Screening, and Scoring, Pfizer Global Research and Development, 2002

Promotions and tenure reviewer for The Scripps Research Institute, University of Michigan, and Georgetown University

Reviewer for manuscripts in Journal of Molecular Biology, Journal of Medicinal Chemistry, Protein Science, Biopolymers, Journal of Computer-Aided Molecular Design, Proteins: Structure, Function, and Genetics, and RECOMB

N.I.H. Computational Biology Study Section, February 2003

D.O.E. Advisory Panel on Computational Protein Structure Prediction, July 2003

Organizer (with Christina Chan, Marianne Huebner, and Helen Geiger), Center for Biological Modeling Annual Retreat and Symposium on Biological Networks, October 2003

Judge, McMaster University High-Throughput Screening and Docking Competition, 2004

Organizer (with Walter Whiteley and Michael Thorpe), Modeling Protein Flexibility and Motions Workshop, Banff, Canada, July 2004

N.I.H. Macromolecular Structure and Function B Study Section, February 2005

Organizer (with Honggao Yan, Richard Lenski, Charles Hoogstraten, and Helen Geiger), Center for Biological Modeling Symposium on the Evolution of Macromolecular Structure, June 2004

Organizer, Midwest Computational Biology Workshop, Augusta, Michigan, April 2005

Organizer (with Michael Feig), Symposium on Modeling Water in Protein-Ligand Interfaces, American Chemical Society National Meeting, Washington, DC, August 2005

N.I.H. Challenges in Docking, Virtual Screening, and Structure-Based Drug Design Summit Meeting, August 2005

Organizer (with Lakshmi Narasimhan and Wan Fang Lau), Symposium on Virtual Screening Using Structure-based and Ligand-based Methods for Lead Identification, American Chemical Society National Meeting, Atlanta, GA, March 26-30, 2006

Organizer (with Peter Bates and Guowei Wei), Midwest Quantitative Biology Conference, Mackinac Island, MI, Sept. 29-Oct. 1, 2006

N.I.H. Research Resource Center Site Visit Member, UCSF, November 2006

Appointed Member, Meridian Township Environmental Commission, May 2008–May 2010

Invited advisor to the scientific review board for the N.I.H. Community Structure Activity Resource (CSAR) Center at the University of Michigan, November 10, 2009

Reviewer, Oak Ridge National Laboratories/Pennsylvania Department of Health Grants, 2008, 2010, 2011, 2013

Editorial Board Member, *Journal of Molecular Recognition*, July 2011–Present

Editorial Board, *Journal of Computer-Aided Molecular Design*, 1999–Present

Coordinator, Mid-Michigan Stewardship Initiative (Ingham, Eaton, Clinton, and Shiawassee County Chapter), The Stewardship Network, October 2008–2013, 2015–Present

Core Team Member, Michigan Invasive Species Coalition, 2012–2013

Director-at-Large and Treasurer, Great Lakes Chapter, Michigan Botanical Club, 2015–2018

University Service

Member, Cell and Molecular Biology Program, 1994–1997

Organizer (with Sakti Pramanik, Michael Thorpe, and William Punch) of MSU Workshop on Computational and Theoretical Biology, April 1999

Organizer (with Bob Cukier) of Workshop on Computational Biology and Bioinformatics in the Michigan Life Sciences Corridor, MSU, November 1999

Co-developer of new joint Ph.D. programs at MSU in Biochemistry & Physics, and Biochemistry & Chemistry with Michael Thorpe and Shelagh Ferguson-Miller, 2000

Chair, MSU Bioinformatics Task Force, Michigan Life Sciences Corridor, 1999–2001

Coordinator (with Michael Thorpe), Computational and Theoretical Sciences Seminar, 1999–2001

Organizer, Center for Biological Modeling Symposium and Retreat, May 2001

Reviewer for IRGP, CDFP, and DFI grant applications at MSU, 2003, 2004, 2010, 2014

Chair, Interdepartmental Computational Biochemistry/Biophysics Faculty Search Committee, 2002–2003

Member, Genetics Program, 2003–Present

Biological Statistics Faculty Search Committee member, 2003–2004 and 2004–2005

College of Osteopathic Medicine Advisory Council Representative for Biochemistry and Molecular Biology, August 2004–2006

Computational Biology Faculty Search Committee member, Dept. of Computer Science and Engineering, 2004–2005

Co-Director, Quantitative Biology and Modeling Initiative, Michigan State University, East Lansing, July 2004–November 2007

Executive Committee, Quantitative Biology Initiative, Michigan State University, East Lansing, December 2007–December 2008
Member, External Review of Promotion and Tenure Committee, Lyman Briggs College, MSU, 2013–2014
Member, Mitchell and Rhodes Scholarship Selection Committee, MSU, 2016
Member, MSUE/MNFI Michigan Vernal Pool Partnership, 2016–2018

Departmental Service

Crystallography Faculty Search Committee, 1994–1995
Coordinator, Biochemistry Colloquium, 1995–1996
Founder and Coordinator, Structural Techniques Seminar, 1995–1999
Search Committee for Computational Specialist, 1996
MSU-IDEA Committee, 1998–2001
Undergraduate Advisor, 1998–2001
Protein Structure, Function, and Design Faculty Search Committee, 1999–2001
Graduate Programs Committee, 1995–1998 (Chair, 1996–1997) and 2003–2004
Search Committee, Biochemistry & Molecular Biology Department Chair, 2006–2007
Faculty Advisory Committee, 1999–2001, Spring 2006, and 2008–2010
Chair, Search Committee for Information Technologist, 2008
Search Committee Member, Structural Biology, 2011
Excellence Search Committee Member, Biochemistry & Molecular Biology, 2011
Comprehensive Exam Organizing Committee, 2010–2013, 2017–2018
Computer Committee, 1994–2011; Chair, 2007–2011, 2013–2015
Undergraduate Advisor, 2012–2013
Awards Committee, 2013–2016; Co-Chair, 2015–2016
Mentoring Committee, 2016–2018
Comprehensive Exam Committee, 2016–2019

Teaching

Instructor, Biochemistry 101, 1998, 2003, 2005, 2008, 2011, and 2014
Coordinator and Instructor, Biochemistry 961, Protein and Ligand Docking, 2011
Instructor, Biochemistry 961/Physics 832/Chemistry 987, Dynamics and Interactions of Proteins and Nucleic Acids, 2007
Coordinator and Instructor, Biochemistry 961, Concepts in Protein Structure (Structural Bioinformatics) Computer Lab, 1996–2001 and Instructor, 2003, 2004, 2006, 2008, 2010, 2012, and 2014
Instructor, Biochemistry 978, Biochemistry Colloquium, 1994–1995 and 2007–2008
Instructor, Biochemistry 495, Senior Seminar/Capstone Course, 1997–1998 and 2003, and Course Coordinator and Instructor, 1999–2001, and 2004–2019
Course Coordinator and Instructor, Biochemistry 803, Protein Structure and Function, 1997–2001, and Instructor, 2003–2011, and 2014–2018
Instructor, Biochemistry 805, Protein Structure, Design, and Mechanism, 2013–2018

Publications

T. G. Frey, L. A. Kuhn, J. S. Leigh, Jr., M. J. Costello and S. H. P. Chan (1985) "Cytochrome Oxidase: Structural Insights from Electron Microscopy and Secondary Structure Prediction", *Journal of Inorganic Biochemistry* **23**, 155-162.

L. A. Kuhn and J. S. Leigh, Jr. (1985) “A Statistical Technique for Predicting Membrane Protein Structure”, *Biochimica et Biophysica Acta* **828**, 351-361.

L. A. Kuhn (1989) “The Prediction and Characterization of Transmembrane Protein Sequences”, Doctoral Dissertation, University of Pennsylvania.

L. A. Kuhn, J. H. Griffin, C. L. Fisher, J. S. Greengard, B. N. Bouma, F. España and J. A. Tainer (1990) “Elucidating the Structural Chemistry of Glycosaminoglycan Recognition by Protein C Inhibitor”, *Proceedings of the National Academy of Sciences USA* **87**, 8506–8510.

J. F. Collawn, M. Stangel, L. A. Kuhn, V. Esekogwu, S. Jing, I. S. Trowbridge, and J. A. Tainer (1990) “Transferrin Receptor Internalization Sequence YXRF Implicates a Tight Turn as the Structural Recognition Motif for Endocytosis”, *Cell* **63**, 1061–1072.

J. F. Collawn, L. A. Kuhn, L.-F. S. Liu, J. A. Tainer, and I. S. Trowbridge (1991) “Transplanted LDL and Mannose-6-Phosphate Receptor Internalization Signals Promote High-Efficiency Endocytosis of the Transferrin Receptor”, *EMBO Journal* **10**, 3247–3253.

L. A. Kuhn, M. A. Siani, M. E. Pique, C. L. Fisher, E. D. Getzoff, and J. A. Tainer (1992) “The Interdependence of Surface Topography and Bound Water Molecules Revealed by Surface Accessibility and Fractal Density Measures”, *J. Mol. Biol.* **228**, 13–22.

M. Boissinot, L. A. Kuhn, P. Lee, C. L. Fisher, Y. Wang, R. A. Hallewell, and J. A. Tainer (1993) “Rational Design and Expression of a Heparin-Targeted Human Superoxide Dismutase”, *Biochem. Biophys. Res. Comm.* **190**, 250–256.

C.-P. Chang, C. S. Lazar, B. J. Walsh, M. Komuro, J. F. Collawn, L. A. Kuhn, J. A. Tainer, I. S. Trowbridge, M. G. Farquhar, M. G. Rosenfeld, H. S. Wiley, and G. N. Gill (1993) “Ligand-induced Internalization of the EGF Receptor is Mediated by Multiple Endocytic Codes Analogous to the Tyrosine Motif Found in Constitutively-internalized Receptors”, *J. Biol. Chem.* **268**, 19312–19320.

L. Pond, L. A. Kuhn, M. R. Jackson, L. Teyton, M.-P. Schutze, J. A. Tainer, and P. A. Peterson (1995) “A Role for Acidic Residues in Di-leucine Motif-based Targeting to the Endocytic Pathway”, *J. Biol. Chem.* **270**, 19989–19997.

L. A. Kuhn and C. L. M. J. Verlinde (1995) “Protein Structure-Based Drug Design”, Fall *American Crystallographic Association Newsletter*, pp. 23–24.

L. A. Kuhn, C. A. Swanson, M. E. Pique, J. A. Tainer, and E. D. Getzoff (1995) “Atomic and Residue Hydrophilicity in the Context of Folded Protein Structures”, *Proteins: Struct. Funct. Genet.*, **23**, 536–547.

M. L. Raymer, W. F. Punch, E. D. Goodman, and L. A. Kuhn (1996) “Genetic Programming for Improved Data Mining–Application to the Biochemistry of Protein Interactions”, *in* Genetic Programming 1996: Proceedings (J. R. Koza, D. E. Goldberg, D. B. Fogel, and R. L. Riolo, eds.), MIT Press, Cambridge, MA, pp. 275–381.

M. L. Raymer, P.C. Sanschagrin, W. F. Punch, S. Venkataraman, E. D. Goodman, and L. A. Kuhn (1997) “Predicting Conserved Water-Mediated and Polar Ligand Interactions in Proteins Using a K-nearest-neighbors Genetic Algorithm”, *J. Mol. Biol.*, **265**, 445–464.

M. L. Raymer, W. F. Punch, E. D. Goodman, P. C. Sanschagrin, and L. A. Kuhn (1997) “Simultaneous Feature Scaling and Selection Using a Genetic Algorithm”, *in* Proceedings of the Seventh International Conference on Genetic Algorithms (T. Bäck, ed.), Morgan Kaufmann Publishers, San Francisco, pp. 561–567 .

L. Craig, P. C. Sanschagrin, A. Rozek, S. Lackie, L. A. Kuhn, and J. K. Scott (1998) “The Role of Structure in Antibody Cross-Reactivity Between Peptides and Folded Proteins”, *J. Mol. Biol.*, **281**, 183-201.

P. C. Sanschagrin and L. A. Kuhn (1998) “Cluster Analysis of Consensus Water Sites in Thrombin and Trypsin Shows Conservation Between Serine Proteases and Contributions to Ligand Specificity”, *Protein Science*, **7**, 2054–2064.

V. Schnecke, C. A. Swanson, E. D. Getzoff, J. A. Tainer, and L. A. Kuhn (1998) "Screening a Peptidyl Database for Potential Ligands to Proteins Including Side-chain Flexibility", *Proteins: Structure, Function, and Genetics*, **33**, 74–87.

V. Schnecke and L. A. Kuhn (1999) "Flexibly Screening for Molecules Interacting with Proteins", *in* Rigidity Theory and Applications (M. F. Thorpe and P. M. Duxbury, eds.), Plenum Publishing, New York, pp. 385–400.

D. Jacobs, L. A. Kuhn, and M. F. Thorpe (1999) "Flexible and Rigid Regions in Proteins", in *Rigidity Theory and Applications* (M. F. Thorpe and P. M. Duxbury, eds.), Plenum Publishing, New York, pp. 357–384.

Q. Yuan, J. J. Pestka, B. M. Hespenheide, L. A. Kuhn, J. E. Linz, and L. P. Hart (1999) "Identification of Mimotope Peptides Which Bind to the Mycotoxin Deoxynivalenol-specific Monoclonal Antibody", *Appl. Environ. Microbiol.* **65**, 3279–3286.

V. Schnecke and L. A. Kuhn (1999) "Database Screening for HIV Protease Ligands: The Influence of Binding-Site Conformation and Representation on Ligand Selectivity", in *Proceedings of the Seventh International Conference on Intelligent Systems for Molecular Biology* (T. Lengauer, R. Schneider, P. Bork, D. Brutlag, J. Glasgow, H.-W. Mewes, and R. Zimmer, eds.), AAAI Press, Menlo Park, CA, pp. 242–251.

B. Essigmann, B. Hespenheide, L. A. Kuhn, and C. Benning (1999) "Prediction of the Active-Site Structure and NAD$^+$ Binding in SQD1, a Protein Essential for Sulfolipid Biosynthesis in *Arabidopsis* ", *Arch. Biochem. Biophys.* **369**, 30–41.

L. Fan, P. C. Sanschagrin, L. S. Kaguni, and L. A. Kuhn (1999) "The Accessory Subunit of Mitochondrial DNA Polymerase Shares Structural Homology with a Domain in Aminoacyl tRNA Synthetases: Implications for a Dual Role as a Primer Recognition Factor and Processivity Clamp", *Proceedings of the National Academy of Sciences, USA* **96**, 9527–9532.

M. F. Thorpe and L. A. Kuhn (1999) "Rigidity in Glasses and Proteins", *Periodica Mathematica Hungarica* **39**, 241–252.

M. F. Thorpe, B. M. Hespenheide, Y. Yang, and L. A. Kuhn (2000) "Flexibility and Critical Hydrogen Bonds in Cytochrome c", *Pacific Symposium on Biocomputing*, eds. R. B. Altman, A. K. Dunker, L. Hunter, K. Lauderdale, & T. Klein, World Scientific, Singapore, pp. 191–205.

M. L. Raymer, W. F. Punch, E. D. Goodman, L. A. Kuhn, and A. K. Jain (2000) "Dimensionality Reduction Using Genetic Algorithms", *IEEE Transactions on Evolutionary Computation* **4**, 164–171.

V. Schnecke and L. A. Kuhn (2000) "Virtual Screening with Solvation and Ligand-Induced Complementarity", *Perspectives in Drug Design and Discovery* **20**, 171–190.

M. F. Thorpe, M. Lei, A. J. Rader, D. J. Jacobs, and L. A. Kuhn (2001) "Protein Flexibility and Dynamics Using Constraint Theory", in *Biological Modeling: Protein Flexibility and Folding* (L. A. Kuhn and M. F. Thorpe, eds.), Elsevier, New York, pp. 60–69.

M. F. Thorpe, M. Lei, A. J. Rader, D. J. Jacobs, and L. A. Kuhn (2001) "Protein Flexibility and Dynamics Using Constraint Theory", *J. Molec. Graphics and Modelling*, **19**, 60–69.

D. J. Jacobs, A. J. Rader, L. A. Kuhn, and M. F. Thorpe (2001) "Protein Flexibility Predictions Using Graph Theory", *Proteins: Structure, Function, and Genetics* **44**, 150–165.

E. E. Howell, U. Shukla, S. N. Hicks, R. D. Smiley, L. A. Kuhn, and M. I. Zavodszky (2001) "One Site Fits Both: A Model for the Ternary Complex of Folate + NADPH in R67 Dihydrofolate Reductase, a D_2 Symmetric Enzyme", *J. Computer-Aided Molec. Design*, **15**, 1035–1052.

M. L. Raymer, L. A. Kuhn, and W. F. Punch (2001) "Knowledge Discovery in Biological Datasets Using a Hybrid Bayes Classifier/Evolutionary Algorithm", *Proceedings of the*

2nd IEEE International Symposium on Bioinformatics and Bioengineering, 236–245.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe (2002) "Protein Unfolding: Rigidity Lost", *Proceedings of the National Academy of Sciences USA* 99, 3540-3545.

B. M. Hespenheide, A. J. Rader, M. F. Thorpe, and L. A. Kuhn (2002) "Identifying protein folding cores from the evolution of flexible regions during unfolding", *J. Molec. Graphics and Modelling*, **21**, 195–207.

M. I. Zavodszky, P. C. Sanschagrin, R. S. Korde, and L. A. Kuhn (2002) "Distilling the Essential Features of a Protein Surface for Improving Protein-Ligand Docking, Scoring, and Virtual Screening", *J. Comp.-Aided Molecular Design*, **16**, 883-902.

B. M. Hespenheide and L. A. Kuhn (2003) "Discovery of a Significant, Non-topological Preference for Antiparallel Alignment of Helices with Parallel Regions in Sheets", *Protein Science*, **12**, 1119–1125.

M. Raymer, T. Doom, L. A. Kuhn, and W. Punch (2003), "Knowledge Discovery in Biological Datasets Using a Hybrid Bayes Classifier/Evolutionary Algorithm", *IEEE Transactions on Systems, Man, and Cybernetics* **33**, 802–813.

M. A. Kron, L. A. Kuhn, P. C. Sanschagrin, M. Hartlein, M. Grotli, and S. Cusack (2003) "Strategies for Anti-filarial Drug Development", *J. Parasitology* **89** (suppl.), S226-S235.

H. Gohlke, L. A. Kuhn, and D. A. Case (2004) "Change in Protein Flexibility Upon Complex Formation: Analysis of Ras-Raf Using Molecular Dynamics and a Molecular Framework Approach", *Proteins: Struct. Funct. Bioinf.* **56**, 322-337.

M. Lei, M. I. Zavodszky, L. A. Kuhn, and M. F. Thorpe (2004) "Sampling Protein Conformations and Pathways", *J. Comp. Chem.* **25**, 1133-1148.

M. I. Zavodszky, M. Lei, A. R. Day, M. F. Thorpe, and L. A. Kuhn (2004) "Modeling Correlated Main-chain Motions in Proteins for Flexible Molecular Recognition", *Proteins: Struct. Funct. Bioinf.* **57**, 243-261.

M. I. Zavodszky and L. A. Kuhn (2005) "Side-Chain Flexibility in Protein-Ligand Binding: The Minimal Rotation Hypothesis", *Protein Science* **14**, 1104-1114.

P.-P. Kung, L. R. Zehnder, J. J. Meng, S. W. Kupchinsky, D. J. Skalitzky, M. C. Johnson, K. A. Maegley, A. Ekker, L. A. Kuhn, P. W. Rose, and L. A. Bloom (2005) "Design, Synthesis, and Biological Evaluation of Novel Human 5'-Deoxy-5'-Methylthioadenosine Phosphorylase (MTAP) Substrates", *Bioorg. Med. Chem. Letters*, **15**, 2829-2833.

M. F. Thorpe, M. Chubynsky, B. Hespenheide, S. Menor, D. J. Jacobs, L. A. Kuhn, M. I. Zavodszky, M. Lei, A. J. Rader and W. Whiteley (2005) "Flexibility in Biomolecules" in *Current Topics in Physics* (R. A. Barrio and K. K. Kaski, eds.), Imperial College Press, London, pp 97–112.

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S. Raschka, A. J. Wolf, J. Bemister-Buffington, and L. A. Kuhn (2018) "Protein-ligand interfaces are polarized: Discovery of a strong trend for intermolecular hydrogen bonds to favor donors on the protein side with implications for predicting and designing ligand complexes", *J. Computer-Aided Molec. Design* 32(4), 511-528.

S. Raschka, A. M. Scott, M. Huertas, W. Li, and L. A. Kuhn (2018) "Automated Inference of Chemical Discriminants of Biological Activity", *in* Methods in Molecular Biology: Computational Drug Discovery and Design (M. Gore and U.B. Jagtap, eds.), Springer Protocols, Humana Press, New York, NY, pp. 307–338 (ISBN (978-1-4939-7755-0).

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L. A. Kuhn (2018) "BioBlitz on Your Own Land", article for Wild Ones Red Cedar Newsletter.

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J. Bemister-Buffington, A. J. Wolf, S. Raschka and L. A. Kuhn (2020) "Machine Learning to Identify Flexibility Signatures of Class A GPCR Activation", *Biomolecules*, 10(3), 454; https://doi.org/10.3390/

J. Chen, L. A. Kuhn, and S. Raschka (2022) "Techniques for Developing Reliable Machine Learning Classifiers Applied to Understanding and Predicting Protein:Protein Interaction Hot Spots" *in* Methods in Molecular Biology: Computational Drug Discovery and Design (M. Gore and U.B. Jagtap, eds.), Springer Protocols, New York, NY, pp. (https://www.biorxiv.org/content/10.1101/2022.12.26.521948v1)

Invited Talks

L. A. Kuhn, M. E. Pique, M. A. Siani, E. D. Getzoff, and J. A. Tainer, "Relating Protein Sequence Patterns to Structural Motifs", talk for the West Coast Protein Crystallography Workshop, Pacific Grove, CA, spring 1991.

L. A. Kuhn, "Decoding and Modifying Protein Structural Recognition Motifs", seminar for Department of Biochemistry and Biophysics, University of Pennsylvania, Philadelphia, PA, August 24, 1992.

L. A. Kuhn, "Using Structural Information from the Protein Data Bank to Design Proteins and Protein Inhibitors", seminar for Department of Chemistry, Simon Fraser University, Burnaby, BC, Canada, February 4, 1993.

L. A. Kuhn, M. E. Pique, C. A. Swanson, M. A. Siani, J. A. Tainer, and E. D. Getzoff, "Protein Hydration and Sequence Patterns in Molecular Recognition", talk for The Scripps Research Institute Faculty Retreat, San Jose del Cabo, Mexico, May 1993.

L. A. Kuhn, "Using Structural Information from the Protein Data Bank to Design Proteins and Protein Inhibitors", talk for Michigan State University Department of Energy Plant Research Laboratory Retreat, Kellogg Biological Station, MI, October 2, 1993.

L. A. Kuhn, "Bound Water's Influence in Structure-Guided Protein and Drug Design", seminar at The Upjohn Company, Kalamazoo, MI, October 17, 1994.

L. A. Kuhn, "Bound Water's Influence in Structure-Guided Protein and Drug Design", seminar at Chiron Corporation, Emeryville, CA, November 10, 1994.

L. A. Kuhn, "Protein and Water Motifs in Molecular Recognition", seminar at Indiana University–Purdue University, Indianapolis, IN, November 28, 1994.

L. A. Kuhn, "The PhD Method for Protein Secondary Structure Prediction", talk for the Michigan State University Structural Techniques Group, January 1995.

L. A. Kuhn, "Shape and Chemical Complementarity in Structure-Based Drug Design", talk for Departments of Chemistry, Molecular Biology, Medicinal Chemistry, and Biology at University of Toledo and Medical College of Ohio, October 1996.

L. A. Kuhn, "Molecular Modeling and Screening for the Design of Protein Ligands", talk for Chugai Biopharmaceuticals, November 1996.

L. A. Kuhn, "Shape and Chemical Complementarity in Structure-Based Drug Design", talk for Structural Bioinformatics, Inc., November 1996.

L. A. Kuhn, "Predicting Water-Mediated Ligand Binding", seminar for Agouron Pharmaceuticals, La Jolla, California, March 1997.

L. A. Kuhn, "The Role of Structure in Antibody Cross-Reactivity Between Proteins and Peptides, and Implications for Vaccine Design", seminar for NSF REU Program, Department of Biochemistry, Michigan State University, East Lansing, July 1997.

L. A. Kuhn and V. Schnecke, “Screening and Docking of Ligands to Protein Active Sites’, talk for the MSU Structural Techniques Group, December 1997.

L. A. Kuhn, “Screening for Potential Ligands to Proteins with Inducible Side-chain Complementarity”, seminar at Pharmacia & Upjohn, Kalamazoo, Michigan, February 1998.

L. A. Kuhn and M. F. Thorpe, “Flexibility in Proteins”, MSU Interdisciplinary Seminar, May 1998.

L. A. Kuhn, “Computing at the Interface Between Molecular Biology, Physics, and Pharmaceutical Chemistry”, seminar for Board of Advisors, MSU College of Natural Science, May 1998

L. A. Kuhn, “Flexibly Screening for Molecules Interacting with Proteins”, talk at Rigidity Theory and Applications conference, Traverse City, Michigan, June 1998.

L. A. Kuhn, “Using Distance Geometry and Hashing for Screening and Docking of Flexible Ligands to Proteins”, seminar for Computational Biology Center, IBM T. J. Watson Research Center, Yorktown Heights, NY, July 1998.

L. A. Kuhn, “Structural Modeling and Design of Proteins and their Interactions”, seminar for the DOE-Plant Research Laboratory, MSU, October 1998.

L. A. Kuhn, “Screening for Peptidyl and Organic Inhibitors of Proteins, Computationally and in Vitro – What Can Be Learned from Combining the Two Approaches?”, seminar for Warner-Lambert Parke-Davis, Ann Arbor, MI, December 1998.

L. A. Kuhn, “Modeling Protein Structures and their Interactions”, seminar for the MSU Biochemistry Club, February 1999.

L. A. Kuhn and V. Schnecke, “Merging Computational and In Vitro Screening for Peptidyl Ligands”, talk at the International Workshop on Virtual Screening, Marburg, Germany, March 1999.

L. A. Kuhn, V. Schnecke, M. L. Raymer, and P. C. Sanschagrin, “How Proteins Fold, Flex, and Bind Other Molecules”, talk for the Workshop on Computational and Theoretical Biology, Michigan State University, April 1999.

L. A. Kuhn, “Decoding Protein Flexibility and Folding from Hydrogen-Bond Networks”, talk for the Workshop on Magnetic Resonance and Optical Imaging Techniques for Biomedical Applications, University of Pennsylvania, May 1999.

L. A. Kuhn and V. Schnecke, “Database Screening for HIV Protease Ligands: The Influence of Binding-Site Conformation on Ligand Selectivity”, talk for the Conference on Intelligent Systems for Molecular Biology, Heidelberg, Germany, July 1999.

L. A. Kuhn, “Modeling Protein and Ligand Flexibility and Binding Site Solvation When Screening Databases for Ligands”, talk for the Gordon Conference on Quantitative Structure Activity Relationships, Tilton, New Hampshire, July 1999.

L. A. Kuhn and V. Schnecke, “SLIDE: Screening for Ligands with Induced-Fit Docking”, seminar at Pharmacia & Upjohn, Kalamazoo, MI, August 1999.

L. A. Kuhn, “Incorporating Flexibility, Solvation, and Molecular Diversity in Ligand Screening”, talk for the American Chemical Society National Meeting, New Orleans, August 1999.

L. A. Kuhn, “New Approaches for Predicting Protein Flexibility and Ligand Interactions”, seminar for the Department of Biochemistry, Michigan State University, August 1999.

L. A. Kuhn, “New Ways of Modeling Protein Flexibility”, talk at Tripos, Inc., St. Louis, October 1999.

L. A. Kuhn, “Screening Large Structural Databases for Diverse Ligands to Flexible, Solvated Proteins”, talk at the Conference on Innovative Applications of Computational Chemistry: The Interface of Library Design, Structure Based Drug Design and Virtual Screening, San Francisco, October 1999.

L. A. Kuhn, “Flexibility in Protein-Ligand Recognition”, talk at the La Jolla Interfaces in

Science Workshop on Quantitative Challenges in the Post-Genomic Sequence Era, San Diego, CA, January 2000.

L. A. Kuhn, "Solvation and Flexibility in Screening for Protein-Ligand Interactions", talk at AstraZeneca, Charnwood, England, January 2000.

L. A. Kuhn, "Computational Screening and Docking of Peptidyl and Organic Ligands to Proteins", seminar for the Institute of Molecular Biology and Biochemistry, Simon Fraser University, Burnaby, British Columbia, February 2000.

L. A. Kuhn, "Modeling Protein Flexibility and Induced Complementarity", seminar for the Department of Biochemistry and Molecular Biology, University of Tennessee, Knoxville, February 2000.

L. A. Kuhn, "Screening and Docking Known and Novel Ligands to the Estrogen Receptor", talk at the EPA conference on Toxicology and Risk Assessment Approaches for the 21st Century, Cincinnati, Ohio, April 2000.

L. A. Kuhn, "A Graph Theory Approach to Predicting Unfolding Pathways of Proteins", talk for *Protein Flexibility and Folding Workshop*, Traverse City, Michigan, August 2000.

L. A. Kuhn, "Molecular Flexibility in Protein Interactions", Physics Colloquium at California State University, Northridge, September 2000.

L. A. Kuhn, "Combinatorial Screening for Protein Ligands", talk at Syrrx, Inc., La Jolla, California, September, 2000.

L. A. Kuhn, "Computationally Screening for Peptidyl and Small Organic Ligands to Flexible, Solvated Proteins", talk for *Informatics Interfaces Symposium* at Pharmacia, Kalamazoo, Michigan, October 2000.

L. A. Kuhn, "More Realistic Modeling of Flexibility and Chemical Complementarity in Structure-Based Screening for Ligands", talk for *Workshop on What Makes a Drug Attractive for its Receptor: ADMET, Affinity and Selectivity*, Marburg, Germany, March 2001.

L. A. Kuhn, "Molecular Flexibility in Drug Design", Interdisciplinary Seminar, MSU, April, 2001

L. A. Kuhn, "Protein Unfolding Pathways and Folding Nucleation Sites Predicted by Graph Theory", talk at workshop on "Protein Folding, Structure, and Design", Trieste, Italy, June 2001.

L. A. Kuhn, "Modeling Protein and Small Molecule Flexibility in Ligand Screening and Docking", talk at the International Workshop on Protein Folding, Structure, and Design, ICTP, Trieste, Italy, June 2001.

L. A. Kuhn, "Modeling Flexibility and Mining the Chemical Determinants of Bioactivity in Small Molecules", talk at Ford Scientific Research Laboratories, Dearborn, Michigan, July 2001.

L. A. Kuhn, P.C. Sanschagrin, M. I. Zavodszky, V. Schnecke, M. Lei, and A. R. Day, "Modeling Large and Small Scale Flexibility of Proteins and Ligands during Screening and Docking", talk at National Meeting of the American Chemical Society, Chicago, August 2001.

L. A. Kuhn, "Modeling Protein Flexibility in Ligand Screening and Docking", talk at Pfizer, La Jolla, September 2001.

L. A. Kuhn, "Modeling Protein Flexibility in Ligand Screening and Docking", talk at University of Michigan Department of Medicinal Chemistry, October 2001.

L. A. Kuhn, "Modeling Protein Flexibility in Ligand Screening and Docking", seminar for the Department of Biochemistry, University of Missouri, Columbia, March 2002.

L. A. Kuhn, "Modeling Protein Flexibility in High-throughput Computational Screening and Docking", talk at Cambridge Healthtech Institute Conference on Structure-Based

Drug Design, Boston, April 2002.

L. A. Kuhn, “Modeling Significant Main-chain Flexibility and Side-chain Induced Fit in Protein-Ligand Docking”, talk at CECAM Workshop on Dynamics of Proteins on a Continuous Energy Landscape, Lyon, France, May 2002.

L. A. Kuhn,“Structure-Based Approaches to Drug Design”, talk for MSU Center for Biological Modeling Annual Symposium, East Lansing, June 2002.

L. A. Kuhn, “Modeling Protein Flexibility in Ligand Docking”, videoseminar to Stanford Biomedical Informatics program, June 2002.

L. A. Kuhn, “Protein Structure-Based Drug Design”, talk at Solid State to Biophysics conference, Dubrovnik, June 2002.

L. A. Kuhn, “Protein Side-chain and Main-chain Flexibility in Ligand Screening and Docking”, talk at Conference on Advances in Structure-Guided Drug Discovery, La Jolla, November 2002.

L. A. Kuhn, “Modeling Protein Flexibility”, talk at Triangle Biophysics Symposium Chapel Hill, North Carolina, November 2002.

L. A. Kuhn, “Protein Allostery”, talk at Workshop on The Geometry of Protein Folding, Holetown, Barbados, January 2003.

L. A. Kuhn, “Balancing Large and Small Scale Flexibility in Protein:Ligand Docking”, talk at American Chemical Society National Meeting, New Orleans, March 2003.

L. A. Kuhn and W. Whiteley, “Rigidity of Geometric Graphs: From Combinatorics to Flexible Proteins”, Combinatorics and Applied Mathematics Seminar, Department of Mathematics, Michigan State University, April 2003.

L. A. Kuhn, “Structural Bioinformatics: Modeling Protein:Ligand Interactions”, Department of Statistics Bioinformatics Seminar, Michigan State University, April 2003.

L. A. Kuhn, “A Unified Approach to Protein-Ligand Flexibility and Docking”, talk at Chemistry-Driven Drug Design and Discovery Conference, San Francisco, June 2003.

L. A. Kuhn, “SLIDE and New Scoring Functions for High-throughput Ligand Screening and Docking”, seminar at Millenium Pharmaceuticals, Boston, August 2003.

L. A. Kuhn, “Deducing Critical Residues in the Folding/Unfolding Transition from the Native Structure”, talk at CECAM Workshop, “Protein Folding: Bringing Theory and Experiment Closer Together”, Lyon, September 2003.

L. A. Kuhn, “Protein Structure-Based Drug Design”, Frontiers in Science Workshop for High School Teachers, East Lansing, September 2003.

L. A. Kuhn, “Feature Selection and Weighting for Predicting Protein Interactions”, seminar for Department of Statistics and Probability, Michigan State University, January 2004.

L. A. Kuhn, “Computational Structural Biology and Biological Modeling Research at MSU” and “Developing Inhibitors and Characterizing Cytokine Activity for Asn tRNA Synthetase in Lymphatic Filariasis”, presentations at the Clinical and Basic Biomedical Research Foci Workshop: Opportunities for Collaboration, Michigan State University, January 2004.

L. A. Kuhn, “High-Throughput Structure-Based Screening to Discover New Protein Ligands”, seminar for Department of Pharmacology and Toxicology, University of Arizona, February 2004.

L. A. Kuhn, “Exploring Protein Flexibility through Bond Networks”, talk at Protein Modelling Workshop, American Mathematical Society Meeting, Lawrenceville, New Jersey, April 2004.

L. A. Kuhn, “Modeling Correlated Main-chain Motion in Proteins and their Ligands”, talk for CECAM Workshop on Flexible Docking, Lyon, France, April 2004.

L. A. Kuhn, “Modeling Flexibility in Protein-Ligand Recognition”, Department of Chemistry, Norwegian University of Science and Technology (NTNU), Trondheim, June

2004.

L. A. Kuhn, “Modeling Protein-Ligand Motions and Interactions in Docking and Screening”, talk at the American Chemical Society 228th National Meeting, Philadelphia, PA, August 2004.

L. A. Kuhn, “Anticipating Protein Flexibility in Inhibitor Binding and Design”, Universite de Montreal Department of Biochemistry, January 24, 2005.

L. A. Kuhn, “Learning from Nature in Modeling Protein Flexibility Upon Ligand Binding”, University of North Carolina Program in Molecular and Cellular Biophysics, Chapel Hill, February 24, 2005.

L. A. Kuhn, “Structure-Based Design of Protein Inhibitors”, Genetics Graduate Program, Michigan State University, March 21, 2005.

L. A. Kuhn, “Using Protein Docking and Flexibility towards Drug Design”, Seminar for Department of Biochemistry and Molecular Biology, Wright State University, Dayton, Ohio, April 1, 2005.

L. A. Kuhn, “Multi-scale Molecular Flexibility in Structure-Based Drug Design”, Contemporary Biochemistry Series, University of Wisconsin, Madison, September 19, 2005.

L. A. Kuhn, “Applying Rigidity Theory to Protein Flexibility and Drug Design”, Engineering Research Brown Bag Seminar, Michigan State University, October 25, 2005.

L. A. Kuhn, “Multiscale Modeling of Protein and Ligand Flexibility Applied to Screening for Novel Inhibitors”, Structure Based Drug Discovery, Keystone Symposium, Whistler, BC, April 4-9, 2006.

L. A. Kuhn, “Structure-based Screening and Flexibility Modeling to Identify Novel Protein Inhibitors”, invited seminar, Biotechnology Research Institute, NRC, Montreal, Canada, May 23, 2006.

L. A. Kuhn, invited lecture, “Docking, Conformational Flexibility, and Drug Design”, invited lecture and lab, EMBO Course on Biomolecular Simulation, Pasteur Institute, Paris, June 28-July 5, 2006.

L. A. Kuhn, invited lectures, “Introduction to Structure-Based Docking and Virtual Screening”, “Representing the Shape, Chemistry, and Flexibility of Proteins and Ligands in Docking”, and “Considerations in Achieving Ligands that are Specific to a Protein Target and Don’t Bind to Homologous Proteins”, Lipari School on Proteomes and Proteins, Lipari Island, Italy, July 9-July 22, 2006.

L. A. Kuhn, invited lecture, “Constraint Counting and Flexibility in Protein Networks”, Midwest Quantitative Biology Conference, Mackinac Island, Michigan, Sept. 29-Oct. 1, 2006.

L. A. Kuhn, invited lecture, “Optimizing Sampling and Scoring in the ASCbase Software for Pocket Mining”, Global Netmeeting, Pfizer Global Research and Development, Ann Arbor, April 30, 2007.

L. A. Kuhn, invited talk, “Optimizing Scoring and Specificity in Screening for Protein Inhibitors”, 4th Annual Indy Bioinformatics Conference, Indianapolis, June 1-2, 2007.

L. A. Kuhn, invited lecture, “Modeling Flexibility in Protein Interactions”, J. W. Goethe University of Frankfurt, Germany, September 19, 2007.

L. A. Kuhn, invited lecture, “Modeling Protein Motions to Maintain Non-Covalent Interactions and Minimize Steric Barriers in Virtual Screening”, Workshop: From Structural Genomics to Drug Discovery: Modelling Flexibility, Parma, Italy, Sept. 20, 2007.

L. A. Kuhn, invited lecture, “Flexibility Modeling in Virtual Screening for Thrombin and Asparaginyl-tRNA Synthetase Inhibitors”, Workshop: From Structural Genomics to Drug Discovery: Modelling Flexibility, Parma, Italy, Sept. 21, 2007.

L. A. Kuhn, invited lecture and lab, EMBO Course on Biomolecular Simulation, Pasteur Institute, Paris, July 2008.

L. A. Kuhn, invited lecture, "Selectivity in structure-based drug design: Tools for identifying similar sites in diverse proteins and pinpointing selectivity determinants", American Chemical Society National Meeting, Philadelphia, PA, August 17-21, 2008

L. A. Kuhn, invited lecture, "Identifying Specificity Determinants in Homologous Proteins and Predicting Ligand Binding Modes for Virtual Screening", Global Netmeeting, Pfizer Global Research and Development, Groton, CT, August 22, 2008

L. A. Kuhn, research overview, "Bioinformatics in the Protein Structural Analysis & Design Lab", Quantitative Biology Initiative Bioinformatics Symposium, MSU, December 13, 2008

L. A. Kuhn, invited lecture, "Adaptive scoring for comparing ligand binding sites and predicting binding modes and affinities", American Chemical Society National Meeting, Salt Lake City, Utah, March 25, 2009

L. A. Kuhn, invited seminar, "The Flow from Docking & Screening into Pocket Mining & Site Hopping", Pfizer Global Research & Development, La Jolla, CA, July 27, 2009

L. A. Kuhn, invited seminar, "ASCbase Update and Kuhn Lab Software Overview", Pfizer Global Research & Development, La Jolla, CA, July 28, 2009

L. A. Kuhn, invited lecture, "Identifying Sites that Bind Similar Ligands in Different Proteins, to Enhance Target-selective Design", Keystone Symposium on Computer-Aided Drug Design, Whistler, BC, April 20–25, 2010

L. A. Kuhn, invited seminar, "Gaining Insights into Ligand Binding and Specificity by Screening Binding Sites for Similarity", Hauptman-Woodward Institute and Structural Biology Department of the School of Medicine and Biomedical Sciences, SUNY Buffalo, Structural Biology in the 21st Century Distinguished Speaker, March 29, 2011

L. A. Kuhn, invited lecture, "How to Mine Protein Flexibility for Inhibitor Selectivity", Great Lakes Bioinformatics Conference, Ann Arbor, May 16, 2012

L. A. Kuhn, invited lecture, "Pocket Mining from Three Points of View: Protein Similarity, Ligand Similarity, and Protein-Ligand Interactions", Dart Neurosciences, San Diego, CA, August 6, 2012

L. A. Kuhn, invited lecture, "Educating Students for an Interdisciplinary World", Experimental Biology 2013/ASBMB, Boston, MA, April 22, 2013.

L. A. Kuhn, invited seminar, "Inhibitor Discovery Using a Trio of Structure-based Screening Techniques", Department of Computational Medicine and Bioinformatics, University of Michigan, Ann Arbor, November 20, 2013.

L. A. Kuhn, invited seminar, "Screening to Identify Pheromone Receptor Antagonists for Invasive Species Control", Department of Entomology, Michigan State University, January 31, 2014.

L. A. Kuhn, N. Liu, A. Scott, S. Gunturu, S. Raschka, M. Huertas, and W. Li, "Screening and Identifying Pheromone Receptor Antagonists for Invasive Species Control", talk for ACS Division of Environmental Chemistry Session:Great Lakes Restoration Initiative: An Environmental Chemistry Challenge", 248th ACS National Meeting and Exposition San Francisco, CA, August 10-14, 2014

L. A. Kuhn, "Small Molecule Docking and Virtual Screening", Molecular Modeling Workshop, Institute for Cyber-Enabled Research, Michigan State University, November 5, 2014

L. A. Kuhn, "How we detect and respond to the world around us: light, adrenaline, and smelling the roses!", Workshop for Grandparents University, Michigan State University, July 2, 2015

L. A. Kuhn, "Japanese Knotweed Control", Stewardship Network national webcast, November 11, 2015

L. A. Kuhn, "Discovery of 3kPZS Pheromone Antagonists for Sea Lamprey Control, invited talk for the Great Lakes Fishery Commission Sea Lamprey Research Board, Ann Arbor, Michigan, March 3, 2016

L. A. Kuhn, S. Raschka, A. Wolf, and J. Bemister-Buffington, "New Signatures of Protein-Small Molecule Binding: Interfacial Rigidity and Polarity", invited talk for the American Chemical Society National Meeting, Symposium on Molecular Recognition: Revealing the Effects Associated with Receptor-Ligand Binding, Washington, D.C., August 20-24, 2017

L. A. Kuhn, "Vernal Pool Citizen Science – 2017 Successes", presentation to the Wild Ones Red Cedar Chapter (native plant society), January 17, 2018

L. A. Kuhn and A. D. Jones, "PFAS in Residential and Food Services", presentation to MSU Auxiliary Services Leadership Team, April 18, 2019

Poster Presentations and Group Members' Talks

L. A. Kuhn and J. S. Leigh, Jr., "A Statistical Technique for Predicting Membrane Protein Structure", poster presented at UCLA Symposium on Protein Structure, Folding and Design, Keystone, Colorado, March 1985.

L. A. Kuhn and J. S. Leigh, Jr., "The Bacteriorhodopsin Puzzle" and "Predicting Membrane Protein Structure", poster presented at Conference on Protein Structure: Molecular and Electronic Reactivity, Philadelphia, Pennsylvania, April 1985.

L. A. Kuhn, A. D. Diehl, and J. S. Leigh, Jr., "Fourier Transform Intensity Matching Classifies Amphiphilic Regions in Protein Sequences", poster presented at Biophysical Society Annual Meeting, San Francisco, California, February 1986.

L. A. Kuhn and J. S. Leigh, Jr., "Characterizing Membrane-Spanning Protein Sequences", poster presented at Conference on Macromolecules, Genes, and Computers, Waterville Valley, New Hampshire, August 1986.

L. A. Kuhn, J. A. Tainer, N. L. Max, and E. D. Getzoff, "Spherical Harmonic Molecular Surfaces", poster presented at Gordon Research Conference on Proteins, New Hampton, New Hampshire, June 1989.

L. A. Kuhn, M. A. Siani, E. D. Getzoff, and J. A. Tainer, "The Solvation of Protein Surfaces", poster presented at AAAS Protein Folding Seminar, New Orleans, Louisiana, February 1990.

L. A. Kuhn, M. A. Siani, E. D. Getzoff, and J. A. Tainer, "Structural and Chemical Affinities of Water Molecules Bound to Protein Surfaces", poster presented at the Protein Society Symposium, San Diego, CA, summer 1990.

L. A. Kuhn, M. E. Pique, M. A. Siani, E. D. Getzoff, and J. A. Tainer, "Identifying Favored Conformations of Amino Acid Sequence Patterns by Searching Known Protein Structures", poster presented at Keystone Symposium on Proteins, Keystone, CO, winter 1991.

L. A. Kuhn, M. A. Siani, E. D. Getzoff, and J. A. Tainer, "The Shape Dependence of Water Binding to Proteins", poster presented at Protein Society Symposium, San Diego, CA, 1992.

L. A. Kuhn, C. A. Swanson, J. A. Tainer, and E. D. Getzoff, "Designing Novel Enzyme Inhibitors from Protein-Solvent Interactions", poster presented at American Cancer Society, California Division, Conference for Postdoctoral Fellows, San Francisco, CA, May 1993.

L. A. Kuhn, M. Boissinot, C. L. Fisher, and J. A. Tainer, "Structure-based Design of Targeted Enzymes", poster presented at the West Coast Protein Crystallography Workshop, Pacific Grove, CA, 1993.

L. A. Kuhn, C. A. Swanson, J. A. Tainer, and E. D. Getzoff, “Using Atomic Crystallographic Hydrophilicity Data to Design Protein Inhibitors”, poster presented at the Protein Society Symposium, San Diego, CA, 1993.

L. A. Kuhn, C. A. Swanson, M. A. Siani, J. A. Tainer, and E. D. Getzoff, “Amino Acid Hydrophobicity in the Context of Folded Proteins: A Crystallographic Hydration Scale”, poster presented at Miami Bio/Technology Winter Symposium, Miami, FL, January 1993.

L. A. Kuhn, W. Y.-J. Chen, C. A. Swanson, E. D. Getzoff, and J. A. Tainer, “Reverse Turn Sequence Motifs for Protein Mutagenesis and Design”, poster presented at the Protein Society Symposium, San Diego, CA, 1994.

L. A. Kuhn, C. A. Swanson, M. E. Pique, J. A. Tainer, and E. D. Getzoff, “Using Atomic Hydrophilicity Measured by Protein Hydration to Evaluate Complementarity in Protein Interfaces”, poster presented at the West Coast Protein Crystallography Workshop, Pacific Grove, CA, spring 1995.

M. L. Raymer, S. Venkataraman, W. F. Punch III, E. D. Goodman, and L. A. Kuhn, “Predicting Conserved Water-Mediated Interactions in Protein Active Sites”, talk for the American Crystallographic Association Annual Meeting, Montreal, Quebec, summer 1995.

M. L. Raymer, L. A. Kuhn, P. C. Sanschagrin, E. D. Goodman, and W. F. Punch III, “Genetic Algorithm Prediction of Water-mediated Ligand Interactions and the Implications for the Chemistry of Water Binding”, invited talk for the Program in Mathematics and Molecular Biology Symposium: From DNA to Protein Structure and Function, Santa Fe, NM, November 1995.

M. L. Raymer, “Learning from Nature: Genetic Algorithms Applied to Protein Recognition”, invited talk for the Michigan State University Structural Techniques Group, January 1996.

L. Craig, L. A. Kuhn, J. S. Mehroke, M. Rashed, L. Bonnycastle, P. C. Sanschagrin, and J. K. Scott, ‘Probing the Basis of Cross-reactivity Between Peptides and Proteins”, poster presented at the International Conference on Protein Folding and Design, National Institutes of Health, Bethesda, MD, April 1996.

L. A. Kuhn, M. L. Raymer, P. C. Sanschagrin, E. D. Goodman, and W. F. Punch III, “Resolving Water-Mediated and Polar Ligand Recognition Using Genetic Algorithms”, poster presented at the International Conference on Protein Folding and Design, National Institutes of Health, Bethesda, MD, April 1996.

M. L. Raymer, “Genetic Programming for Improved Data Mining – Application to the Biochemistry of Protein Interactions”, poster presented at Genetic Programming 1996, Stanford University, Palo Alto, CA, July 1996.

L. A. Kuhn, M. L. Raymer, W. F. Punch III, P. C. Sanschagrin, and E. D. Getzoff, “Predicting and Analyzing Determinants of Water-Mediated Ligand Recognition”, poster presented at the International Union of Crystallography XVII Congress, Seattle, WA, August 1996.

M. L. Raymer, “Computational Protein Folding with Chaperones – The Current State of the Art”, invited talk for the MSU Structural Techniques Group, November 1996.

P. C. Sanschagrin, M. L. Raymer, and L. A. Kuhn, “Cluster Analysis of Multiple Serine Protease Structures Identifies Conserved Water Sites Involved in Structure and Specificity”, poster presented at the West Coast Protein Crystallography Workshop, Pacific Grove, California, March 1997.

L. A. Kuhn, “Predicting Water-Mediated Recognition”, poster presented at National Academy of Sciences Colloquium on Computational Biomolecular Sciences, Newport Beach, CA, 1997.

L. A. Kuhn, P. C. Sanschagrin, and M. L. Raymer, "Using Cluster Analysis to Identify Conserved Binding Sites in Proteins", poster presentation at Protein Society Symposium, Boston, Massachusetts, July 1997.

M. L. Raymer, W. F. Punch, E. D. Goodman, P. C. Sanschagrin, and L. A. Kuhn, "Simultaneous Feature Extraction and Selection Using a Masking Genetic Algorithm", talk at the Seventh International Conference on Genetic Algorithms, July 1997.

L. Craig, P. C. Sanschagrin, A. Rozek, L. A. Kuhn, and J. K. Scott, "The Role of Structure in Cross-Reactivity Between Peptides and Folded Proteins", poster presentation at Protein Society Symposium, Boston, Massachusetts, July 1997.

M. L. Raymer, W. F. Punch, P. C. Sanschagrin, E. D. Goodman, and L. A. Kuhn, "Discovering the Chemistry of Conserved First-Shell and Active-Site Hydration in Proteins Using Pattern Classification with a Genetic Algorithm", poster presentation at Protein Society Symposium, Boston, Massachusetts, July 1997.

V. Schnecke and L. A. Kuhn, "Screening Databases for Potential Ligands to Protein Active Sites", poster presentation at Protein Society Symposium, Boston, Massachusetts, July 1997.

M. L. Raymer, W. F. Punch, E. D. Goodman, P. C. Sanschagrin, and L. A. Kuhn, "Simultaneous Feature Extraction and Selection Using a Masking Genetic Algorithm", invited talk at the Seventh International Conference on Genetic Algorithms, July 1997.

L. A. Kuhn, W. B. Anderson, C. E. Barkham, M. L. Raymer, and P. C. Sanschagrin, "Implications of Structural Comparison of Prostaglandin Synthase Isozymes and Ribonucleotide Reductase for Understanding their Specificity and Catalysis", poster presentation at American Heart Association, Michigan Affiliate Cardiovascular Research Forum, Ann Arbor, September 1997.

V. Schnecke and L. A. Kuhn, "Screening and Docking of Ligands to Protein Active Sites', invited talk for the MSU Structural Techniques Group, December 1997.

V. Schnecke and L. A. Kuhn, "Screening for Potential Ligands to Proteins with Inducible Side-chain Complementarity", poster presentation at UCSF/MDI Conference on Molecular Recognition in Drug Design: Docking and Scoring, San Francisco, California, February 1998.

M. L. Raymer, P. C. Sanschagrin, W. F. Punch, E. D. Goodman, and L. A. Kuhn, "Elucidating the Determinants of Conserved Protein Surface Solvation Using a Genetic Algorithm and Nearest Neighbor Classifier", poster presentation at UCSF/MDI Conference on Molecular Recognition in Drug Design: Docking and Scoring, San Francisco, California, February 1998.

D. J. Jacobs, M. F. Thorpe, and L. A. Kuhn, "Identifying Floppy and Rigid Regions in Proteins", talk at the American Physical Society Meeting, Los Angeles, CA, March 1998.

B. Essigmann, L. A. Kuhn, R. M. Garavito, and C. Benning, "Biochemical Characterization, Crystallization, and Structural Modeling of the SQD1 Protein Involved in Sulfolipid Biosynthesis of Arabidopsis thaliana", poster presentation at the 9th International Conference on Arabidopsis Research, Madison, WI, June 1998.

L. A. Kuhn and B. M. Hespenheide, "Favored Secondary Structural Interactions as a Guide to Protein Folding", poster presentation to the Twelfth Symposium of the Protein Society, San Diego, CA, July 1998.

M. L. Raymer, P. C. Sanschagrin, and L. A. Kuhn, "Identifying the Determinants of Conserved Protein Solvation", poster presentation to the Twelfth Symposium of the Protein Society, San Diego, CA, July 1998.

V. Schnecke and L. A. Kuhn, "Screening for Flexible Ligands with Solvation and Conformational Change of the Protein Binding Site", poster presentation to the Twelfth

Symposium of the Protein Society, San Diego, CA, July 1998.

P. C. Sanschagrin and L. A. Kuhn, "The Contributions of Conserved Bound Water Molecules to Thrombin and Trypsin Structure and Specificity", poster presentation to the Cardiovascular Research Forum, American Heart Association, Michigan Affiliate, Detroit, MI, October 1998.

L. A. Kuhn and V. Schnecke, "Representing Induced Complementarity of Protein, Ligand, and Solvent While Screening for Peptidyl and Organic Ligands", poster presentation to the Pacific Symposium on Biocomputing, Mauna Lani, Hawaii, January 1999.

L. A. Kuhn, M. L. Raymer, P. C. Sanschagrin, E. D. Goodman, and W. F. Punch III, "The Nature of Protein-Water Interactions", poster presentation at N.S.F. Career Awardees Symposium, Washington, DC, January 1999.

L. Fan, P. C. Sanschagrin, L. A. Kuhn, and L. S. Kaguni, "Structural Model of the Accessory Subunit of Pol Gamma", talk at the Keystone Symposium on Molecular Mechanisms of DNA Replication and Recombination, February 1999.

D. J. Jacobs, L. A. Kuhn, and M. F. Thorpe, "Flexibility and Rigidity in Protein Structures", talk at the American Physical Society Centennial Meeting, Atlanta Georgia, March 1999.

V. Schnecke and L. A. Kuhn, "Screening and Docking of Flexible Organic Ligands to Solvated Binding Sites with Induced Complementarity", poster presentation to the Workshop on Virtual Screening, Marburg, Germany, March 1999.

D. J. Jacobs, L. A. Kuhn, and M. F. Thorpe, "Predicting Conformational Flexibility in Protein Structure", talk at the American Physical Society meeting on Industrial and Applied Physics, May 1999.

A. J. Rader, D. J. Jacobs, M. F. Thorpe, and L. A. Kuhn, "Rigid and Flexible Regions in Proteins", poster presentation at the 13th Annual MSU Center for Fundamental Materials Research Symposium, 1999.

P. C. Sanschagrin, L. Fan, L. S. Kaguni, and L. A. Kuhn, "Threading and Structural Analysis of a Novel DNA Polymerase Subunit Indicates Roles in Primer Recognition and Processivity", poster presentation at the Thirteenth Symposium of the Protein Society, Boston, July 1999.

V. Schnecke and L. A. Kuhn, "Database Screening for HIV Protease Ligands: The Influence of Binding-Site Conformation on Ligand Selectivity", invited talk for the Conference on Intelligent Systems for Molecular Biology, Heidelberg, Germany, July 1999.

B. M. Hespenheide, M. F. Thorpe, and L. A. Kuhn, "Hydrogen Bond Networks in Protein Flexibility and Folding", poster presentation to the Thirteenth Symposium of the Protein Society, Boston, July 1999.

A. J. Rader, L. A. Kuhn, and M. F. Thorpe, "Ligand Binding Effects on Protein Rigidity and Flexibility", poster presented at the 47th Annual Midwest Solid State Conference, Ohio University, 1999.

M. F. Thorpe and L. A. Kuhn, "Rigidity in Proteins and Glasses", invited talk for the Fourth Geometry Festival, An International Workshop on Discrete Geometry and Rigidity, Budapest, Hungary, December 1999.

L. A. Kuhn, V. Schnecke, and P. C. Sanschagrin, "Predicting Which Ligands Bind to a Protein, and Where", poster presented at Pacific Symposium on Biocomputing, Honolulu, HI, January 2000.

B. M. Hespenheide, M. F. Thorpe, and L. A. Kuhn, "Protein Flexibility and Folding Pathways", poster presented at the La Jolla Interfaces in Science Workshop on Quantitative Challenges in the Post-Genomic Sequence Era, San Diego, CA, January 2000.

A. J. Rader, L. A. Kuhn, and M. F. Thorpe, "Prediction of Protein Flexibility", poster presented at the La Jolla Interfaces in Science Workshop on Quantitative Challenges in the Post-Genomic Sequence Era, San Diego, California, January 2000.

A. J. Rader, L. A. Kuhn, and M. F. Thorpe, “Computational Detection and Analysis of Protein Flexibility”, poster presented at the 14th Annual MSU Center for Fundamental Materials Research Symposium, February 2000.

A. J. Rader, L. A. Kuhn, B. M. Hespenheide, and M. F. Thorpe, “The Transition Between Rigidity and Flexibility in Proteins and Glasses”, poster presentation for *Protein Flexibility and Folding Workshop*, Traverse City, Michigan, August 2000.

M. I. Zavodszky, P. C. Sanschagrin, and L. A. Kuhn, “Induced Fit in Database Screening”, poster presentation for *Protein Flexibility and Folding Workshop*, Traverse City, Michigan, August 2000.

B. M. Hespenheide, M. F. Thorpe, and L. A. Kuhn, “Protein Flexibility and Unfolding Pathways”, poster presentation for *Protein Flexibility and Folding Workshop*, Traverse City, Michigan, August 2000.

H. Krishnamurthy, A. J. Rader, M. F. Thorpe, L. A. Kuhn, J. G. Zeikus, and C. Vieille, “Testing FIRST Predictions on Protein Stability Using Adenylate Kinase as a Model System”, poster presentation for *Protein Flexibility and Folding Workshop*, Traverse City, Michigan, August 2000; J. Molecular Graphics and Modeling 18(4), 551.

M. Lei, L. A. Kuhn, and M. F. Thorpe, “Constrained Dynamics of the Flexible Regions in Proteins”, poster presentation for *Protein Flexibility and Folding Workshop*, Traverse City, Michigan, August 2000; J. Molecular Graphics and Modeling 18(4), 551.

P. C. Sanschagrin, M. I. Zavodszky, and L. A. Kuhn, “Template-Based Computational Screening for Ligands Including Side-chain Flexibility and Interfacial Solvent”, poster presentation for *Intelligent Systems for Molecular Biology*, San Diego, California, August 2000.

A. J. Rader, “The Protein Folding Problem”, talk for MSU Condensed Matter Physics Brown Bag Seminar, October 2000.

M. I. Zavodszky, P. C. Sanschagrin, and L. A. Kuhn, “Realistic Modeling of Polar Interactions in Ligand Screening”, poster presentation at *Workshop on What Makes a Drug Attractive for its Receptor: ADMET, Affinity and Selectivity*, Marburg, Germany, March 2001.

P. C. Sanschagrin, M. I. Zavodszky, and L. A. Kuhn, “Modeling of Hydrophobic Interactions in Computational Ligand Screening: A Template Matching Approach”, *Workshop on What Makes a Drug Attractive for its Receptor: ADMET, Affinity and Selectivity*, Marburg, Germany, March 2001.

M. F. Thorpe and L. A. Kuhn, “Floppy Modes and Rigidity in Network Glasses and in Proteins”, invited talk at the International Workshop on Disordered Systems, Andalo, Italy, March 2001.

A. J. Rader, L. A. Kuhn, and M. F. Thorpe, “Protein Unfolding: An Example of a Rigid-Floppy Phase Transition”, poster presentation at the MSU Center for Fundamental Materials Research Symposium, spring 2001.

A. R. Day, M. Lei, M. F. Thorpe, and L. A. Kuhn, “Modeling the Flexibility of Ring Molecules in Structure-Based Screening for Ligands”, poster presentation at the Center for Biological Modeling Annual Retreat, Augusta, Michigan, May 2001.

B. M. Hespenheide, M. F. Thorpe, and L. A. Kuhn, “Identifying the Initiation Sites of Protein Folding Using FIRST Flexibility Analysis”, poster presentation at the Center for Biological Modeling Annual Retreat, Augusta, Michigan, May 2001.

M. Lei, A. R. Day, L. A. Kuhn, and M. F. Thorpe, “Constrained Dynamics of the Flexible Regions in Proteins”, poster presentation at the Center for Biological Modeling Annual Retreat, Augusta, Michigan, May 2001.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe, “Protein Unfolding: Rigidity Lost?", poster presentation at the Center for Biological Modeling Annual Retreat, Augusta, Michigan, May 2001.

P. C. Sanschagrin, M. I. Zavodszky, V. Schnecke, and L. A. Kuhn, "Modeling of Hydrophobic Interactions in Computational Ligand Screening: A Template Matching Approach", poster presentation at the Center for Biological Modeling Annual Retreat, Augusta, Michigan, May 2001.

M. I. Zavodszky, P. C. Sanschagrin, and L. A. Kuhn, "Realistic Modeling of Polar Interactions in Ligand Screening", poster presented at the Center for Biological Modeling Annual Retreat, Augusta, Michigan, May 2001.

B. M. Hespenheide, A. J. Rader, M. F. Thorpe, and L. A. Kuhn, "Protein Folding Cores Identified Using FIRST Flexibility Analysis", poster presented at the International Workshop on Protein Folding, Structure and Design, ICTP, Trieste, Italy, June 2001.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe, "Protein Unfolding: Rigidity Lost?", poster presented at the International Workshop on Protein Folding, Structure and Design, ICTP, Trieste, Italy, June 2001.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe, "Protein Unfolding: Rigidity Lost", talk for MSU CMP Brown Bag Seminar, September, 2001.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe, "The Mean Coordination, $<r>$, as a Protein Folding Reaction Coordinate", poster at the 16th Annual MSU Center for Fundamental Materials Research Symposium, April 2002.

B. M. Hespenheide, A. J. Rader, M. F. Thorpe, and L. A. Kuhn, "Structural Characterization of Protein Unfolding Pathways", poster presented at the MSU Center for Biological Modeling Annual Symposium, East Lansing, June 2002.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe, "Protein Unfolding Driven by Changing Mean Coordination", poster presented at the MSU Center for Biological Modeling Annual Symposium, June 2002.

M. Lei, M. I. Zavodszky, A. Roy Day, L. A. Kuhn, and M. F. Thorpe, "Rigidity Optimised Constrained Kinetics to Explore Protein Conformational Space", poster presented at the MSU Center for Biological Modeling Annual Symposium, June 2002.

M. I. Zavodszky and L. A. Kuhn, "New Ligands Identified for Thrombin by Virtual Screening", poster presented at the MSU Center for Biological Modeling Annual Symposium, June 2002.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe, "Protein Unfolding Driven by Changing Mean Coordination" poster presented at the Protein Society Symposium, San Diego, California, August 2002.

B. M. Hespenheide, A. J. Rader, M. F. Thorpe, and L. A. Kuhn, "Structural Characterization of Protein Unfolding Pathways", poster presented at the Protein Society Symposium, San Diego, CA, August 2002.

M. I. Zavodszky, M. Lei, M. F. Thorpe, and L. A. Kuhn, "Modeling protein main-chain flexibility in ligand docking and screening", poster presented at the Protein Society Symposium, San Diego, CA, August 2002.

M. Lei, M. I. Zavodszky, A. R. Day, L. A. Kuhn, and M. F. Thorpe, "Rigidity Optimised Constrained Kinetics to Explore Protein Conformational Space", poster presented at the Protein Society Symposium, San Diego, CA, August 2002.

A. Hendrick, L. A. Kuhn, J. Leykam, M. Hartlein, and M. Kron, "Design of Peptides for Improved Tropical Disease Diagnosis", poster presented at Minority Research Forum, San Diego, CA, March 2003.

A. J. Rader, B. M. Hespenheide, L. A. Kuhn, and M. F. Thorpe, "Protein Unfolding: Rigidity Lost", poster presented at the American Physical Society Annual Meeting, March 2003.

M. I. Zavodszky, “Modeling Flexibility in Molecular Recognition”, invited talk at Canadian Computational Chemistry Conference, July 2003.

T. Crepin, M. Kron, L. Kuhn, M. Grotli, M. Härtlein, and S. Cusack, “Design of Macrofilaricidal Aminoacyl-tRNA Synthetase Inhibitors”, poster presented at the 10th Annual tRNA Workshop, Banz, Germany, October 2003.

L. A. Kuhn, P. C. Sanschagrin, S. C. K. Sukuru, S. Cusack, and M. A. Kron, “Discovery of New tRNA Synthetase Inhibitors by Structure-Based Screening”, poster presented at the 10th Annual tRNA Workshop, Banz, Germany, October 2003.

A. Stumpff-Kane and L. A. Kuhn, “FIRST: Determining the Steps in Protein Folding”, poster presented at MSU Center for Biological Modeling Symposium on the Evolution of Biomolecular Structure, East Lansing, MI, June 2004.

L. He, M. I. Zavodszky, and L. A. Kuhn, “Empirical Scoring Functions in Structure-Based Molecular Screening and Docking”, poster presented at MSU Center for Biological Modeling Symposium on the Evolution of Biomolecular Structure, East Lansing, MI, June 2004.

S. Arora, W. Punch, P. Duxbury, and L. A. Kuhn, “Optimizing Hydrogen-bond Networks in Protein-Ligand Interfaces”, poster presented at MSU Center for Biological Modeling Symposium on the Evolution of Biomolecular Structure, East Lansing, MI, June 2004.

S. C. K. Sukuru, Y. P. Milev, F. Danel, M. G. P. Page, J. C. Morris, M. Grotli, M. A. Kron and L. A. Kuhn, “Structure-Based Screening and Design for tRNA Synthetase Inhibitors”, poster presented at MSU Center for Biological Modeling Symposium on the Evolution of Biomolecular Structure, East Lansing, MI, June 2004.

M. I. Zavodszky, “Modeling Flexibility in Molecular Recognition”, invited talk at Modeling Protein Flexibility and Motions Workshop, Banff, Canada, July 2004.

C. Sukuru, S. Arora, M. I. Zavodszky, M. Kron and L. A. Kuhn, “Flexible Protein Structure-Based Screening and Docking: Applications to Anti-Filarial Drug Design”, poster at 18th Protein Society Symposium, San Diego, CA, August 2004.

M. Zavodszky, invited talk, Arizona State University Biophysics, November 2004.

S. C. K. Sukuru, T. Crepin, J. C. Morris, M. Grotli, F. Danel, M. G. P. Page, S. Cusack, M. A. Kron, and L. A. Kuhn, “Structural Determinants of Brugia malayi Asparaginyl tRNA Synthetase Affinity and Specificity for Inhibitors Discovered by Structure-Based Screening”, poster at Quantitative Biology and Modeling Symposium, Michigan State University, April 2005.

M. I. Zavodszky, M. Lei, M. F. Thorpe, and L. A. Kuhn, “Modeling Flexibility in Molecular Recognition”, poster at Quantitative Biology and Modeling Symposium, Michigan State University, April 2005.

S. C. K. Sukuru, T. Crepin, J. C. Morris, M. Grotli, F. Danel, M. G. P. Page, S. Cusack, M. A. Kron, and L. A. Kuhn, “Structural Determinants of Brugia malayi Asparaginyl tRNA Synthetase Affinity and Specificity for Inhibitors Discovered by Structure-Based Screening”, poster at Midwest Computational Structural Biology Workshop, Augusta, Michigan, April 2005.

M. I. Zavodszky, M. Lei, M. F. Thorpe, and L. A. Kuhn, “Modeling Flexibility in Molecular Recognition”, invited talk at Midwest Computational Structural Biology Workshop, Augusta Michigan, April 2005.

S. Arora, W. Punch, P. Duxbury, and L. A. Kuhn, “Optimizing Hydrogen-bond Networks in Protein-Ligand Interfaces”, poster presented at MSU Computer Science and Engineering Poster Session, winning First Prize in Algorithms and Theory category, April 2005.

M. I. Zavodszky and L. A. Kuhn, “Side-chain Flexibility at Protein-protein and Protein-ligand Interfaces”, poster presented at 3rd Conference on Modeling of Protein Interactions in Genomes", Lawrence, KS, June 26-28, 2005.

T. A. Mueller, M. I. Zavodszky, M. Feig, L. A. Kuhn, and R. P. Hausinger, "Insights into the enantiospecificities of (R)- and (S)-dichlorprop-ketoglutarate dioxygenases", 12th International Conference on Biological Inorganic Chemistry, Ann Arbor, MI, July 2005.

S. C. K. Sukuru, T. Crepin, J. C. Morris, M. Grotli, F. Danel, M. G. P. Page, S. Cusack, M. Hartlein, M. A. Kron, and L. A. Kuhn, "The Contributions of Conformational Flexibility to Brugia malayi Asparaginyl-tRNA Synthetase Specificity for Inhibitors Identified by Structure-Based Screening", poster for the American Chemical Society National Meeting, Atlanta, GA, March 2006.

A. Rohatgi, S. C. K. Sukuru, Y. Milev, M. Kron, and L. A. Kuhn, "Computational Screening of Sigma Aldrich and NCI Compounds to Discover Inhibitors of Brugia malayi Asparaginyl-tRNA Synthetase", poster for the Michigan State University Undergraduate Research and Arts Forum, winning First Place in Biochemistry, April 7, 2006.

D. Canella, L. A. Kuhn, and M. F. Thomashow, "Understanding CBF Protein Activity through the Study of Two Evolutionarily Conserved Sequences", poster for Plant Biology 2006, East Lansing, MI, July 2006.

S. C. K. Sukuru, T. Crepin, J. C. Morris, M. Grotli, F. Danel, M. G. P. Page, S. Cusack, M. Hartlein, M. A. Kron, and L. A. Kuhn, "Analyzing Water Sites in Class II Aminoacyl tRNA Synthetase Structures for Structure-Based Design of Selective Inhibitors", poster for Quantitative Biology and Modeling Initiative Poster Session, Michigan State University, East Lansing, MI, August 21, 2006.

J. Van Voorst and L. A. Kuhn, "Finding the Optimal Alignment for Labeled 3D Point Sets Describing Surfaces: Applications to Comparing Protein Binding Sites", poster for Quantitative Biology and Modeling Initiative Poster Session, Michigan State University, East Lansing, MI, August 21, 2006.

M. Tonero, M. I. Zavodszky, and L. A. Kuhn, "Improving Scoring Functions that Predict Protein-Ligand Interactions in SLIDE and the Application to Species Selective Drug Screening", poster for Quantitative Biology and Modeling Initiative Poster Session, Michigan State University, East Lansing, MI, August 21, 2006.

J. Van Voorst, L. Narasimhan, and L. A. Kuhn, "Finding the Optimal Alignment for Labeled 3D Point Sets Describing Surfaces: Applications to Comparing Protein Binding Sites", poster for Midwest Quantitative Biology Conference, Mackinac Island, MI, September 29-October 1, 2006

C. Sukuru and L. A. Kuhn, "A Geometric Method for Defining Binding Site Chemistry and Specificity Differences Between Similar Proteins: Applied to Adenosyl Sites", oral presentation for Drug Discovery session at American Chemical Society National Meeting, Chicago, IL, March 2007.

J. Van Voorst, M. E. Tonero, L. Narasimhan, and L. A. Kuhn, "Comparing Protein Binding Sites by Alignment of Favored Positions for Hydrogen-Bond and Hydrophobic Interactions Sites", poster for Indy Regional Bioinformatics Conference, IUPUI Conference Center, Indianapolis, May 31-June 2, 2007.

M. E. Tonero, M. I. Zavodszky and L. A. Kuhn, "Improving Scoring Functions that Predict Protein-Ligand Interactions in SLIDE", poster for Indy Regional Bioinformatics Conference, IUPUI Conference Center, Indianapolis, May 31-June 2, 2007.

M. E. Tonero, M. I. Zavodszky, and L. A. Kuhn, "Novel Scoring Metric for Enhancing the Prediction of Ligand Binding Mode", oral presentation for American Chemical Society National Meeting, Philadelphia, PA, August 17-21, 2008

J. R. Van Voorst and L. A. Kuhn, "Screening Ligand Binding Site Fragments", oral presentation for American Chemical Society National Meeting, Philadelphia, PA, August 17-21, 2008

J. R. Van Voorst and L. A. Kuhn, "Pocket Mining with ASCbase", oral presentation for Pfizer Global Research and Development, Groton, CT, August 22, 2008

L. A. Kuhn, V. Randall, and J. Greenway (2009) "The Mid-Michigan Stewardship Initiative", poster for The Stewardship Network's Science, Practice & Art of Restoring Ecosystems Conference, East Lansing, MI, January 2009.

M. E. Tonero and L. A. Kuhn, "Hydrophobic Complementarity: A Dominant Term in Affinity and Binding Mode Prediction", oral presentation, American Chemical Society National Meeting, Boston, MA, August 2010

C. Reidy, L. A. Kuhn, and S. Thomas,"The Flora of Lake Lansing Park North, Ingham County, Michigan", poster for The Stewardship Network's Science, Practice & Art of Restoring Ecosystems Conference, East Lansing, MI, January 2011.

L. A. Kuhn, N. Sanchez, L. Kaufman, P. Witte, C. Lambertini, W. Guo, and L. Meyerson, "Controlling Introduced Phragmites and Japanese Knotweed while Protecting Native Phragmites in the Lake Lansing Watershed", poster for The Stewardship Network's Science, Practice & Art of Restoring Ecosystems Conference, East Lansing, MI, January 2012.

L. Buhrow, S. Ferguson-Miller, and L. Kuhn, "From Static Structure to Living, Breathing Protein: Computational Analysis of Cytochrome c Oxidase Main-chain Flexibility", poster for Biophysical Society Meeting, February 2012

L. Buhrow, S. Ferguson-Miller, and L. Kuhn, "From Static Structure to Living, Breathing Protein: Computational Analysis of Cytochrome c Oxidase Main-chain Flexibility", poster for ASBMB Special Symposium on Mitochondria: Energy, Signaling, and Homeostasis, East Lansing, MI, June 27-29, 2012, *Best Poster Award*

L. Buhrow, C. Hiser, J. Van Voorst, S. Ferguson-Miller and L. Kuhn, "Three-Pronged Computational Prediction and in vitro Confirmation of Cytochrome c Oxidase Steroid-Binding Site Specific Ligands", poster for Biophysical Society Meeting, February 2013

B. Atshaves, J. Lwande, C. Najt, S. Gupta, K. Moon, A. McIntosh, and L. Kuhn, "Characterization of the ADRP Fatty Acid Binding Site: A Fluorescence Binding and Circular Dichroic Study", abstract for ASBMB/Experimental Biology 2013, Boston, MA, April 2013

L. Kaufman, L. A. Kuhn, and N. Sanchez, "Engaging the Public in Native Plant Gardening and Restoration through Demonstration Gardens", poster for The Stewardship Network's Science, Practice & Art of Restoring Ecosystems Conference, East Lansing, MI, January 2013.

S. Gunturu, A. Scott, M. Huertas, W. Li, and L. A. Kuhn, "Discovery of 3kPZS Antagonists for Sea Lamprey Control", poster for Biochemistry and Molecular Biology Undergraduate Poster Session, MSU, April 19, 2013. Winner of Michigan Society of Toxicology Poster Prize.

J. Bemister, W. Li, and L. A. Kuhn, "Assigning Function to New Receptor Sequences", Honors Chemistry Laboratory Poster Session (Chemistry 186H), MSU, April 25, 2013.

C. P. Najt, J. Lwande, A. L. McIntosh, S. Senthivinayagam, K. Moon, S. Gupta, L. A. Kuhn, and B. P. Atshaves, "Characterization of the Plin2 Lipid Binding Site by Molecular Modeling, Fluorescence Binding, Circular Dichroism, and FRET Studies", poster for 2013 American Society for Biochemistry and Molecular Biology Annual Meeting, Boston, MA, April 22, 2013.

N. Liu, J. R. Van Voorst, and L. A. Kuhn, "CholMine: A Tool to Detect Cholesterol and Cholate Binding Sites in Membrane and Soluble Proteins", poster for American Chemical Society National Meeting, Computers in Chemistry Division, Indianapolis, IN, September 2013.

N. Liu, J. R. Van Voorst, and L. A. Kuhn, "CholMine: A Tool to Detect Cholesterol and

Cholate Binding Sites in Membrane and Soluble Proteins", poster for MSU Department of Biochemistry and Molecular Biology Retreat, Bengel Nature Center, Bath, MI, September 21, 2013.

A. Scott, M. Huertas, N. Liu, S. Gunturu, L. A. Kuhn, and W. Li, "Development of Pheromone Antagonists for Sea Lamprey Control", poster for Neuroscience 2013, San Diego, CA, November 2013.

R. Roston, L. A. Kuhn and C. Benning, "A family I galactosyl hydrolase performs galactosyltransferase activity requiring Mg2+ and conferring freezing tolerance", poster for ASBMB Annual Meeting, San Diego, CA, April 2014.

L. Chaturvedi, K. Sun, M. Walsh, L. A. Kuhn and M. Basson, "The P-loop region of Schlafen 3 acts within the cytosol to induce differentiation of human Caco-2 intestinal epithelial cells", abstract for Digestive Disease Week, May 2014, Chicago, IL; Gastroenterology 146(5), S-785-785.

E. Boerman and L. A. Kuhn, "Inhibiting Myrosinase in *Alliaria petiolata*", poster presentation for the University Undergraduate Research and Arts Forum, Michigan State University, East Lansing, MI April 4, 2014

E. Boerman and L. A. Kuhn, "Inhibiting Myrosinase in *Alliaria petiolata*: A novel method for invasive species control", poster presentation for the Honors Chemistry Lab (CEM186), Michigan State University, East Lansing, MI April 24, 2014

A. Scott, M. Huertas, N. Liu, S. Gunturu, S. Raschka, L. A. Kuhn, and W. Li, "Identification of pheromone receptor antagonists for invasive sea lamprey control", poster for the International Congress on the Biology of Fish, Heriot-Watt University, UK, 3–7 August, 2014

S. Raschka, N. Liu, S. Gunturu, A.M. Scott, M. Huertas, W. Li and L.A. Kuhn, "A Hypothesis-Driven Virtual Screening Methodology for Structure-Based Inhibitor Discovery", poster presentation for Quantitative Biology Symposium, Michigan State University, East Lansing, August 18, 2014

N. Liu, "Two Routes to Ligand Discovery", seminar for the Physical Chemistry Division, Department of Chemistry, Michigan State University, November 24, 2014.

S. Raschka, "Practical Data Science - An Introduction to Predictive Modeling, Machine Learning, and Pattern Classification", oral presentation for the Institute for Cyber-Enabled Research, Michigan State University, Feb. 11, 2015.

B. Zeng, S. Wang, N. Xi, L. A. Kuhn and M. D. Basson,"Inhibition of Pressure-Stimulated FAK and Akt1 Interaction via a 33 Amino Acid FAK-derived Peptide", poster presentation for Digestive Disease Week, Washington, DC, May 16–19, 2015

M. D. Basson, L. Chaturvedi, K. Sun, P. Kovalenko, L. A. Kuhn, and M. Walsh,"Schlafen 12 regulates human enterocyte differentiation by binding to serpin B12", poster presentation for Digestive Disease Week, Washington, DC, May 16–19, 2015; Gastroenterology 148(4), S-8.

A. Scott, M. Huertas, S. Raschka, N. Liu, L. A. Kuhn, and W. Li, "Regulation of Pheromone Induced Responses with Behavioral Antagonists for Invasive Sea Lamprey (Petromyzon marinus L.) Control", poster presentation for Behaviour 2015 conference, Cairns, Australia, August 8, 2015.

A. M. Scott, S. D. Fissette, S. Raschka, L. A. Kuhn, and W. Li, "An Update on the Identification of Sea Lamprey Pheromones and Antagonists", oral presentation for Sea Lamprey Annual Workshop, Traverse City, Michigan. February 3-4, 2016.

S. Raschka, "A Novel Approach to Protein-Ligand Binding Mode Prediction by Using Rigidity Theory", oral presentation for the BioMolecular Science Gateway Graduate Program, Michigan State University, East Lansing, MI, Feb. 8, 2016

S. Raschka, "Screenlamp: A Software Framework for Hypothesis-Driven Ligand Discovery Based on Virtual Screening and Machine Learning", poster for Great Lakes Bioinformatics and Canadian Computational Biology Conference 2016, University of Toronto, May 16–19, 2016

S. Gula, V. M. Lopez, L. A. Kuhn, J. Francese, D. J. Crook, M. D. Ginzel, and A. M. Ray, "Response of adult Anoplophora glabripennis (Coleoptera: Cerambycidae) to host-derived isothiocyanates", poster presentation for the International Conference of Entomology, Orlando, FL, Sept. 25–30, 2016

S. Raschka, "Detecting the Native Ligand Orientation by Interfacial Rigidity", oral presentation for Department of Biochemistry and Molecular Biology Retreat, Okemos, MI, Oct. 7, 2016

A. M. Scott, S. Raschka, L. A. Kuhn, W. Li, "Identification of Novel Sea Lamprey Pheromones & Pheromone Antagonists", oral presentation for BEACON Chemical Communication Group, Michigan State University, East Lansing, MI, Nov. 15, 2016.

A. M. Scott, S. Raschka, L. A. Kuhn, and W. Li, "Discovery of Pheromone Antagonists for Sea Lamprey Control", oral presentation for the Great Lakes Fishery Commission Sea Lamprey Research Board, Ann Arbor, MI, Jan. 20, 2017.

A. M. Scott, M. Huertas, S. Raschka, N. Liu, L. A. Kuhn, and W. Li, "Exploitation of pheromone induced responses with behavioral antagonists for invasive sea lamprey (Petromyzon marinus L.) control", poster presentation for Ecology, Evolutionary Biology, and Behavior Program, Michigan State University, East Lansing, MI, Feb. 3, 2017.

A. M. Scott, S. Raschka, L. A. Kuhn, and W. Li, "Research Update", oral presentation for Sea Lamprey Trapping and Barrier Task Force Meeting, Ann Arbor, MI, Feb. 21, 2017.

S. Raschka, "Protein-Ligand Docking and Ligand-Based Virtual Screening", oral presentation for Computational Biology Journal Club, Michigan State University, Mar. 21, 2017.

S. Gula, L. A. Kuhn, A. M. Ray, and M. Ginzel, "Response of adult Anoplophora glabripennis (Coleoptera: Cerambycidae) to isothiocyanates", oral presentation at Entomological Society of America North Central Meeting, Indianapolis, IN, June 4-7, 2017

S. Raschka, "Screenlamp and BioPandas", oral presentation at SciPy, Austin, TX, Jul. 12, 2017.

A. M. Scott, S. Raschka, L. A. Kuhn, and W. Li, "Sea lamprey attractant pheromones and antagonists research highlights", oral presentation for U.S. Congressional Tour, Hammond Bay Biological Station, Millersburg, MI, Oct. 17, 2017.

S. Raschka, "Building hypothesis-driven virtual screening pipelines for millions of molecules", oral presentation at Open Data Science Conference West, San Francisco, CA, Nov. 2–5, 2017

S. Raschka, "Uncovering Hidden Patterns of Molecular Recognition", Ph.D. Dissertation seminar, Dec. 13, 2017, Michigan State University

C. P. Borowsky, S. Raschka, and L. A. Kuhn, "Base-Pair-Like Hydrogen Bond Patterns Contribute to Specificity in Protein-Ligand Complexes", University Undergraduate Research and Arts Forum, Michigan State University, April 5, 2019

C. P. Borowsky, S. Raschka, and L. A. Kuhn, "DNA Base-Pair-Like Hydrogen Bond Patterns Contribute to Specificity in Protein-Ligand Complexes", Lyman Briggs College Research Symposium, Michigan State University, April 22-25, 2019